FLUX-CORRECTED TRANSPORT TECHNIQUES FOR TRANSIENT CALCULATIONS OF STRONGLY SHOCKED FLOWS

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SUMMARY

New flux-corrected transport algorithms are described for solving generalized continuity equations. These techniques were developed by requiring that the finite-difference formulae used ensure positivity for an initially positive convected quantity. Thus FCT is particularly valuable for fluid-like problems with strong gradients or shocks. Repeated application of the same subroutine to mass, momentum, and energy conservation equations gives a simple solution of the coupled time-dependent equations of ideal compressible fluid dynamics without introducing an artificial viscosity. FCT algorithms span Eulerian, sliding-rezone, and Lagrangian finite-difference grids in several coordinate systems. The latest FCT techniques are fully vectorized for parallel/pipeline processing and are being used on the Texas Instruments ASC at NRL.

INTRODUCTION

This paper reviews the Flux-Correct Transport (FCT) techniques which have been developed to solve the continuity equation

$$\frac{\partial \rho}{\partial t} = - \underline{\nabla} \cdot \rho \underline{V} \qquad \text{(conservation form).} \tag{1a}$$

In addition to (1a), there are two other ways to write the continuity equation which get reflected in some of the numerical solution techniques:

$$\underbrace{\frac{\partial \rho}{\partial t} + \underline{V} \cdot \underline{\nabla} \rho}_{\text{convection}} = \frac{d\rho}{dt} = \underbrace{-\rho \nabla \cdot V}_{\text{compression}}, \qquad \text{and} \tag{1b}$$

(convection form)

$$\frac{\partial}{\partial t} \int_{\text{region}} \rho d^3r = - \oint_{\text{region boundary}} \rho \underline{V} \, d\underline{A} \quad . \tag{1c}$$

(integral form)

The convective term $\underline{V} \cdot \underline{\nabla} \rho$ displayed explicity in Eq. (1b) gives (1a-c) its intrinsically hyperbolic form and causes really severe problems numerically. The compression term - $\rho\underline{\nabla}\cdot\underline{V}$ is sometimes absent, as in the Liouville Equation, in which case it is often called the convection or the advection equation.

Continuity equations underlay compressible and incompressible fluid dynamics, hydrodynamics, plasma physics (Vlasov Equation and MHD moment equations) and even quantum mechanics. They appear in most descriptions of dynamic physical systems simply because they express two of the more general principles in physics, conservation and causality. Continuity equations also display the positivity property: a quantity being transported will never turn negative anywhere in a reasonable flow field if that quantity was everwhere positive to start with. This positivity property expresses in a continuum way the intrinsic corpuscular nature of matter. Thus matter cannot be removed from a region which is devoid of matter to begin with. This duality, in which matter obeys both particle and fluid-like equations on microscopic and macroscopic scales respectively, has its ramifications for numerical solution techniques as well. The first three of the possible solution techniques listed below take advantage of the underlying discrete basis of the continuity equation while the last three aim more directly at solving the partial differential equation itself.

TABLE 1 - Possible Solution Techniques

- Quasiparticle Methods
  1. Collisionless particles, stars and plasmas
  2. Collisional particles for fluids
- Characteristic Methods
- Lagrangian Finite Difference Methods
- Eulerian Finite Difference Methods
  1. Explicit vs implicit
  2. Order vs accuracy
- The Finite Element Method
- The Spectral Method

Because of their speed and simplicity, finite-difference solutions of the continuity equation must always be considered carefully as the most likely of the six candidate methods (ref 1). Quoting three conclusions in a similar context from another source (ref 2):

- The spectral method has no stability problems but is much more complicated and slower than generalized difference methods.
- It is doubtful whether the finite-element method, based on piecewise polynomials, can compete with the above methods.

- If difference methods are used, they should be at least fourth-order accurate.

While I agree basically with these remarks, they do not really encompass the quasiparticle schemes nor do they adequately reflect a very important piece of personal experience. Whenever a theory is to be tested, or an algorithm, or a new mathematical technique, attention rather quickly turns to the crucial yet simple conservation equations of ideal compressible flow.

Finite-difference methods have solved the transient Rankine-Hugoniot shock problem adequately. For that matter, various flavors of quasiparticle methods can do the same vital problem creditably if enough particles are used. I do not know of any calculation, even in one spatial dimension, using either a finite-element or a spectral method which has correctly solved for an ideal gas compressible shock. Until such calculations become common place and computationally attractive, finite-difference methods would seem to have the inside track.

IMPROVING FINITE-DIFFERENCE TECHNIQUES

There is undoubtedly some merit in trying to boost the performance of quasiparticle methods on the one hand and the basis-function expansion methods on the other toward the performance obtained from finite differences. But it is a low risk-high return investment to patch up the obvious failings of the front runners, finite differences. In the case of Lagrangian finite-difference methods, the major outstanding problems arise from secularly unattractive distortions of the grid which wreck calculations of interesting flows quite quickly (refs. 3,4,5). In the case of Eulerian methods, the major outstanding weakness in a hugh class of problems of real interest is the need for a large artificial damping (numerical diffusion) to fill in what would otherwise be pits of "negative density" in the calculated profiles. Since the "Eulerian" positivity problem is encountered even in Lagrangian calculations for many situations, it demands the greater share of attention.

The Flux-Corrected Transport techniques (FCT) which are the subject of this paper have been designed carefully to satisfy the following six requirements of an "ideal" algorithm for solving the continuity equation (ref. 6-9). An ideal algorithm should:

1. Be linearly stable for all cases of interest,
2. Mirror conservation properties of the physics,
3. Ensure the positivity property when appropriate,
4. Be reasonably accurate,
5. Be computationally efficient, and
6. Be independent of specific properties of one application.

FCT algorithms arise naturally (ref 6) as a result of trying to satisfy requirement 3. Most work in the past has centered on trying to increase the mathematical order of accuracy of a scheme while ignoring the physical positivity property which the fluids display prominently.

Consider the rather general three-point approximation to Eq. (1a)

$$\tilde{\rho}_j = \rho_j^o - \frac{1}{2}\left(\rho_{j+1}^o + \rho_j^o\right)\epsilon_{j+1/2} + \frac{1}{2}\left(\rho_j^o + \rho_{j-1}^o\right)\epsilon_{j-1/2}$$
$$+ \nu_{j+1/2}\left(\rho_{j+1}^o - \rho_j^o\right) - \nu_{j-1/2}\left(\rho_j^o - \rho_{j-1}^o\right) , \tag{2}$$

where $\epsilon_{j+1/2} \equiv V_{j+1/2}\delta t/\delta X_{j+1/2}$ and ρ_j is the density at mesh point j. Equation (2) is in finite-difference conservative form with whole indices representing cell centers and half indices indicating cell interfaces. The additional numerical diffusion terms with diffusion coefficients $\nu_{j+1/2}$ have to be added to ensure positivity. The stability of Eq. (2) is ensured, at least roughly, when

$$\frac{1}{2} > \nu_{j+1/2} > \frac{1}{2}\epsilon_{j+1/2}^2 . \tag{3a}$$

The upper limit arises from the explicit diffusion time-step condition while the lower limit is the Lax-Wendroff damping. Unfortunately positivity is only ensured linearly when

$$\nu_{j+1/2} > \frac{1}{2}\left|\epsilon_{j+1/2}\right| , \tag{3b}$$

the first-order upstream-centered scheme result.

We appear to be caught between a rock and a hard place here but the escape route is signaled in the preceding sentence by the word "linearly". By relaxing the linearity implied by Eq. (2) and letting the diffusion coefficients be nonlinear functionals of the flow velocities $\left\{\epsilon_{j+1/2}\right\}$, we can hope to reduce the integrated dissipation below the rather ghastly limit (3b) and yet retain sufficient dissipation near steep gradients to ensure positivity. A literature is beginning to form about these "monotonic" difference schemes (refs. 6-9, 10, 11) since the dilemma of accuracy versus positivity in Eulerian difference schemes can be resolved in no other way.

FLUX-CORRECTED TRANSPORT ALGORITHMS

The first, and so far the most developed and used, of the monotonic schemes is Flux-Corrected Transport. The calculation in Fig. 1 was performed by the first FCT Algorithm SHASTA (ref. 7) and had an error about four or five times smaller than the simple linear methods also shown. The damping was second order as were the relative phase errors. Figure 1 shows a comparison of four common difference schemes solving the standard square wave problem. The effects of excess numerical damping in the donor-cell treatment (upstream-centered first-order), and of excess dispersion in the leap frog and Lax-Wendroff treatments are clearly visible. Dispersion manifests itself as a trail or projection of oscillations in the computed solution near discontinuities and sharp gradients of the "correct" solution.

The basic FCT technique shown in Figure 1 was quickly generalized to cylindrical and spherical systems, to Lagrangian as well as fixed Eulerian grids, and was applied to a number of one-, two-, and three-dimensional problems. More recent work has been devoted toward extending the basic nonlinear flux-correction techniques to convection algorithms other than SHASTA and toward discovering an "optimum" FCT algorithm.

Since the latest FCT algorithms have eliminated roughly 95% of the removable error and the removable error that remains is barely half of the irreducible error, it is natural to have turned next toward optimization in speed, flexibility, and generality (ref. 12). In Flux-Corrected Transport algorithms, the basic convective transport algorithm is augmented with a strong enough linear diffusion to ensure positivity at the expense of excess smoothing. Since the amount of diffusion which has been added is known, FCT then performs a conservative antidiffusion step to remove the diffusion in excess of the stability limit. However, the antidiffusive fluxes are effectively multiplied by a coefficient which ranges from zero to unity to preserve monotonicity. The criterion for choosing the reduction factors of the antidiffusive fluxes is that the antidiffused solution will exhibit no new maxima or minima where the diffused solution had none.

Although the limit (3b) represents the minimum amount of diffusion needed for stability, FCT algorithms generally use a larger zero-order diffusion because it has been found that the correct choice of the $\{\nu_{j+1/2}\}$ within the monotonic and stable range will reduce convective phase errors from second to fourth order as suggested by Kreiss. Since the antidiffusion can also be chosen correspondingly larger, no real price is exacted for this improvement in phase properties. The most recent efforts (ref. 12) have taken advantage of this fact to generate minimum-operation-count FCT algorithms for Cartesian, cylindrical, and spherical coordinate systems with stationary (Eulerian) and moveable (Lagrangian) grid systems. Because these algorithms, and in particular the nonlinear flux-correction formula, were very carefully designed, they are fully "vectorizeable" for pipeline and parallel processing and have been implemented in all generality in Fortran on the Texas Instruments Advanced Scientific Computer at the Naval Research Laboratory. The execution time per continuity equation per grid point is roughly 1.3 μsec. A complete 2D calculation on a system of 200 grid points X200 grid points requires roughly 2 to 2.5 seconds per timestep depending on extra physics and boundary conditions incorporated in the problem.

Figure 2 shows a 1D calculation performed by the code FAST1D on the ASC. The problem chosen is the "Lapidus" problem (ref. 13) in cylindrical coordinates with $\gamma = 1.4$. The diaphragm is originally at r - 1.0 in Fig. 2 and bursts at t - 0.0 sec. The density solution is shown at 0.6 sec in Fig. 2 just after the shock has reached the axis and rebounded. Three different resolution calculations are overlapped to show the convergence. Even the calculation with 50 cells is at least as accurate as the original Payne and Lapidus solutions with 200 cells. The width of the contact discontinuity is about 3.5 cells while the shock is smeared over only 1.5 cells without noticeable overshooting or undershooting. The calculations are performed without any added artificial viscosity. The monotonicity control provided by FCT on each of the continuity equations separately is adequate to ensure stability and accuracy as shown.

Figures 3a, b show the evolution of Rayleigh-Taylor instability in the implosion of a laser pellet shell 30 microns thick. The calculation was performed using the FAST2D code on the ASC and the thermal conductivity was set to zero to show the full nonlinear evolution of the instability. An Eulerian "sliding-rezone" grid was used with 200 X 200 grid points. Strong deterioration of the shell is apparent by 3.85 nsec but breakthrough has not yet occurred. The jetting of material off the backside is severe enough by this time that grid distortion would obviate the usual Lagrangian solution techniques. Figure 3a shows the linear phase of the instability and 3b shows the onset of the nonlinear regime.

REFERENCES

1. Boris, J. P.: Numerical Solution of Continuity Equations. Proceedings of the 2nd European Conference on Computational Physics, Garching 27-30 April 1976.

2. Kreiss, H. O.: A Comparison of Numerical Methods Used in Atmospheric and Oceanographic Applications. in Proc. of the Symposium on Numerical Models of Ocean Circulation, National Academy of Sciences (U.S.G.P.O., Washington, D.C., 1972). See also in the same volume B. Wendroff, Problems of Accuracy with Conventional Finite-Difference Methods and G. Fix, A Survey of Numerical Methods for Selected Problems in Continuum Mechanics.

3. Boris, J. P., Fritts, M. J. and Hain, Klaus: Free Surface Hydrodynamics Using a Lagrangian Triangular Mesh. Proc. First Int'l Conference on Numerical Ship Hydrodynamics, NBS, Gaitherburg, Md. Oct 1975.

4. Fritts, M. J.: A Numerical Study of Free-Surface Waves. SAI Report SAI-76-528-WA, March 1976.

5. Chan, R.: A Generalized Arbitrary Lagrangian-Eulerian Method For Incompressible Flows with Sharp Interfaces. J. Comput. Phys. 17(3), pp. 311-331 (1974). See also Hirt, Amsden and Cook, J. Comput. Phys. 14, pp. 227-253 (1974).

6. Boris, J. P. and Book, D. L.: Solution of Continuity Equations by the Method of Flux Corrected Transport. Chap. 11 in Methods in Computational Physics, Vol. 16 (Academic Press, New York, 1976).

7. Boris, J. P. and Book, D. L.: Flux-Corrected Transport I: SHASTA-A Fluid Transport Algorithm that Works. J. Comput. Phys. 11, p. 38ff (1973). [FCT I]

8. Book, D. L., Boris, J. P., Hain, K. H.: Flux-Corrected Transport II: Generalizations of the Method. J. Comput. Phys. 18(3), pp. 248-283 (1975). [FCT II]

9. Boris, J. P. and Book, D. L.: Flux-Corrected Transport III: Minimal Error FCT Algorithms. J. Comput. Phys. 20, (1976). [FCT III]

10. VanLeer, B.: Toward the Ultimate Conservative Difference Scheme. J. Comput. Phys. 14, 361-370 (1974).

11. Harten, A.: The Method of Artificial Compression. CIMS Report COO-3077-50, June 1974.

12. Boris, J. P.: Flux-Corrected Transport Modules for Generalized Continuity Equations. NRL Memorandum Report 3237, 1976 (to be published).

13. Lapidus, A.: Computation of Radially Symmetric Shocked Flows. J. Comput. Phys. 8, pp. 106-118 (1971).

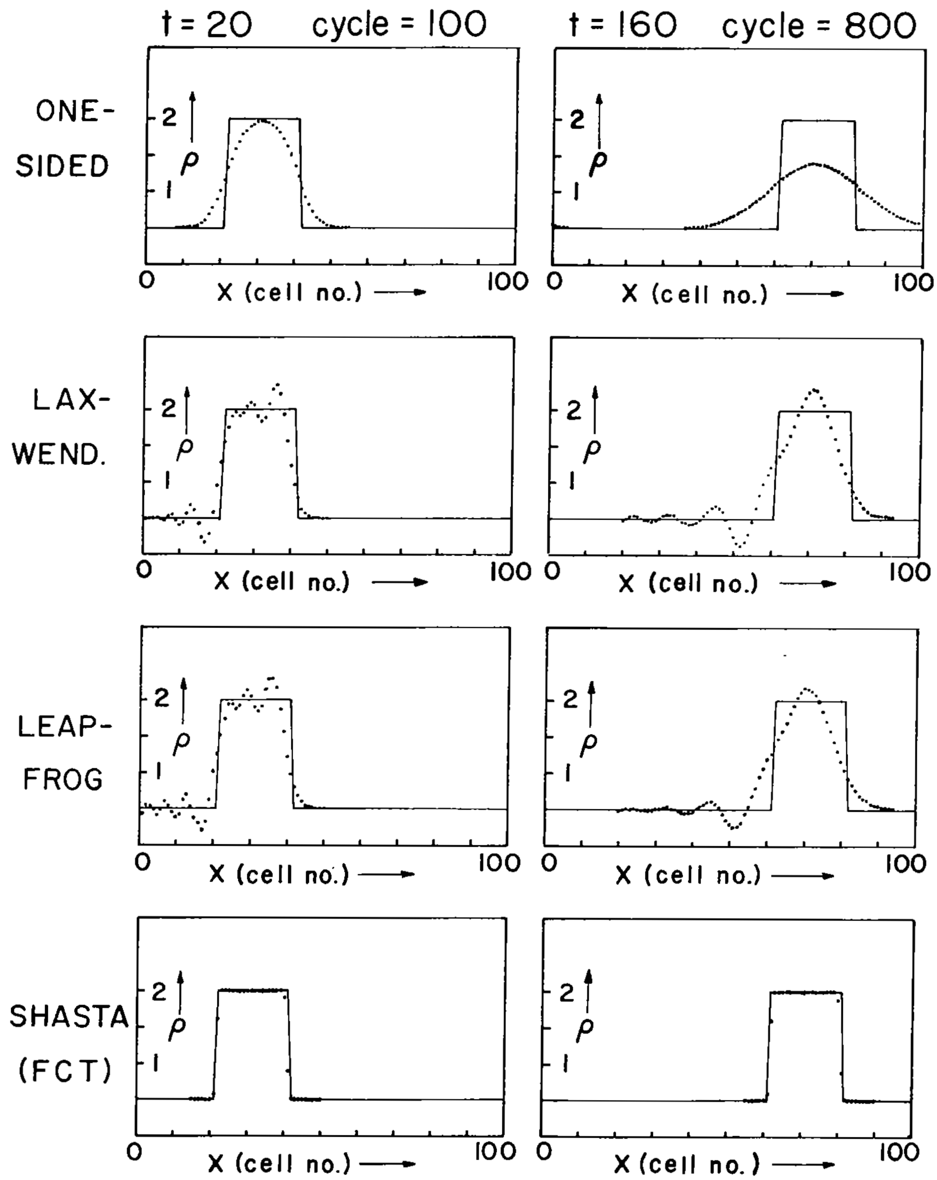


Figure 1.- Comparison of four difference schemes solving the square wave problem. The merits of Flux-Corrected Transport relative to the other methods are clear.

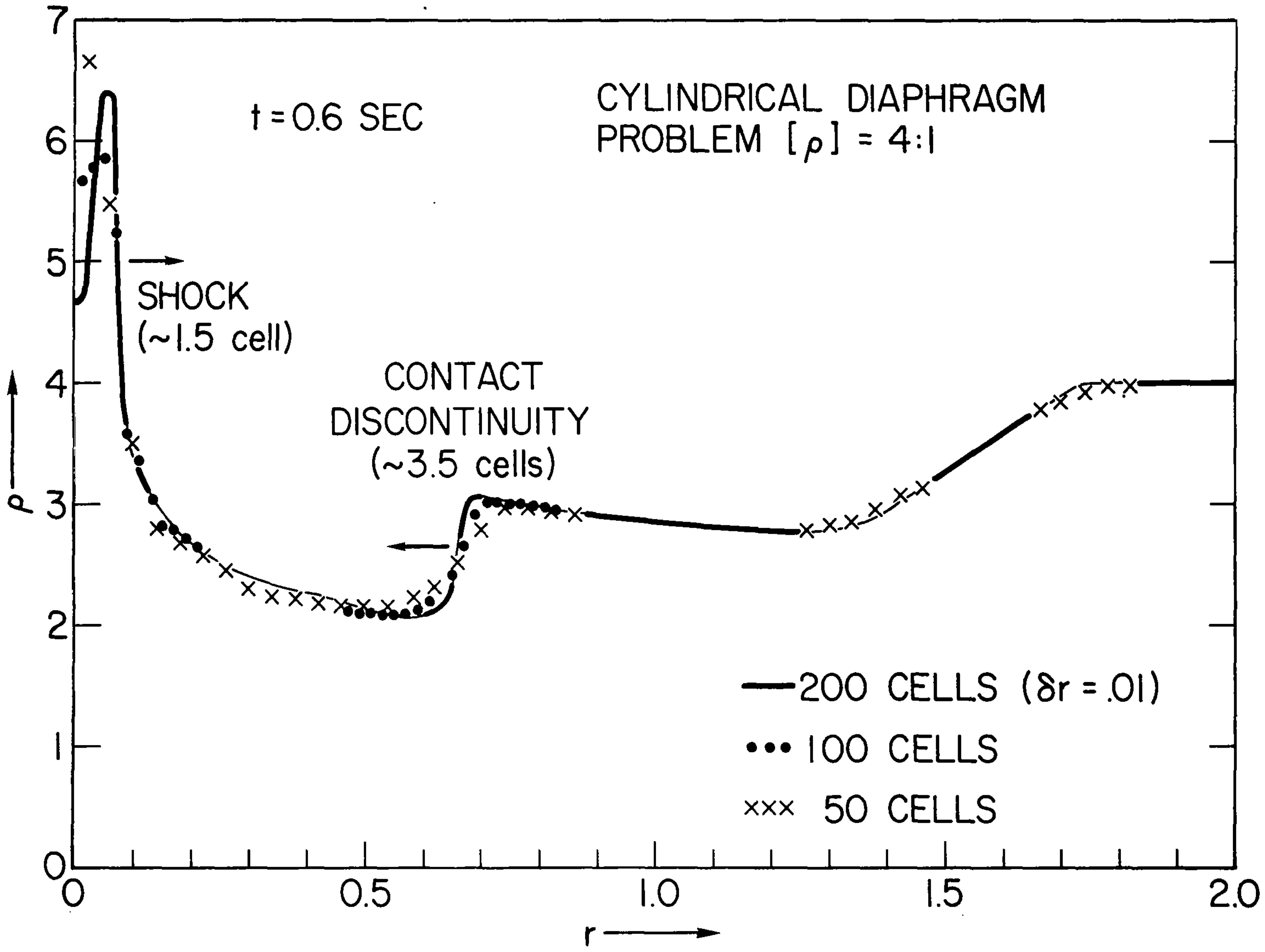
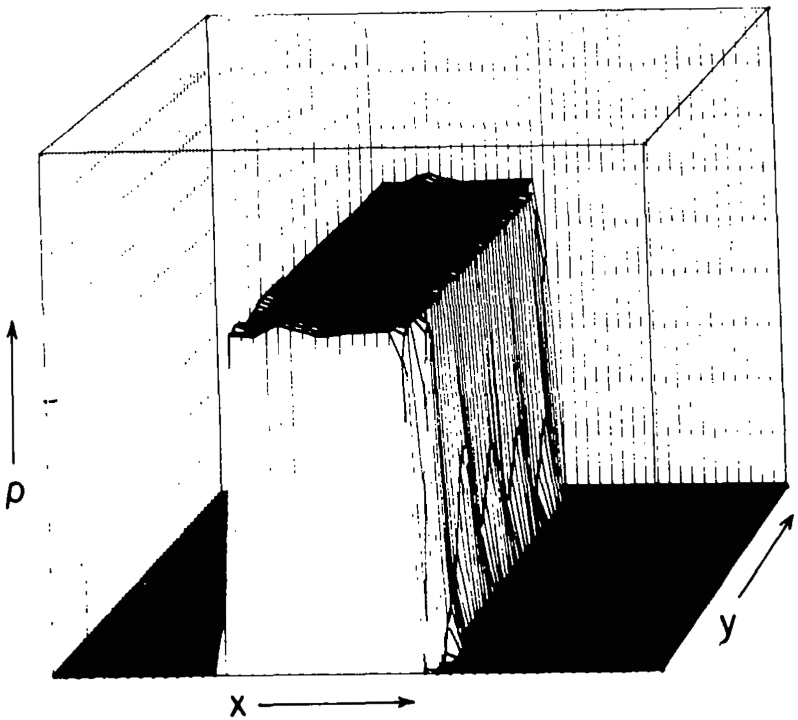
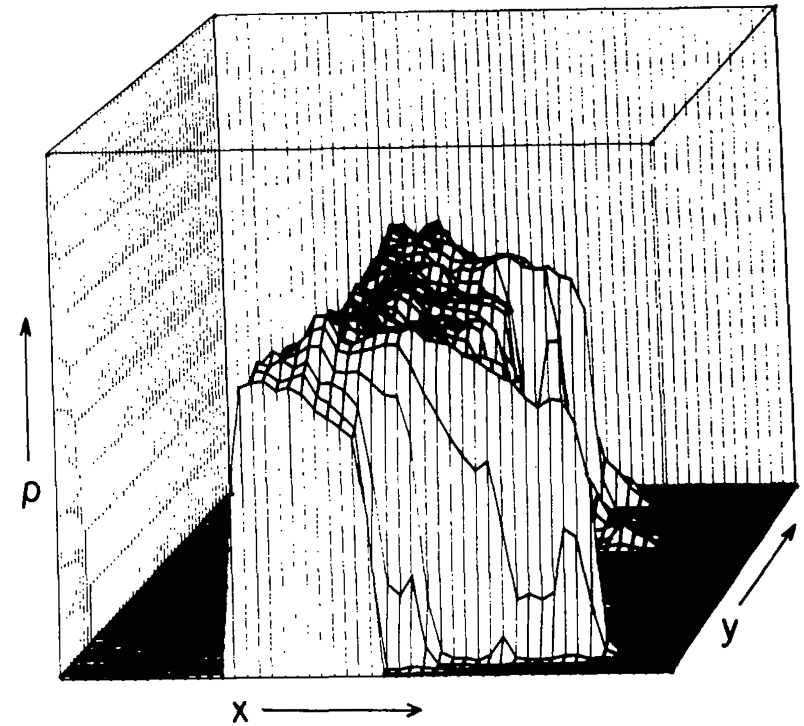


Figure 2.- A cylindrical diaphragm problem using FAST1D. Three different resolutions are shown to demonstrate convergence of the solution. FCT generally requires shock widths of about 1.5 cells.



(a) After 1.05 nsec the beginnings of the Rayleigh-Taylor instability can be seen in the linear phase on the back side of the shell.



(b) After 3.85 nsec the shell has moved roughly two shell thicknesses and the Rayleigh-Taylor instability is fully developed. Usual Lagrangian treatments would be breaking down here because of severe grid distortion.

Figure 3.- Two plots from a FAST2D calculation of a laser pellet shell being imploded (toward the left) by a strong constant pressure (high temperature) on the right showing the nonlinear evolution of the Rayleigh-Taylor instability. The shell is 30 microns thick with an initial density of 3 gg/cc.